COMPUTING A RESIDUE FINGERPRINT FOR A MOLECULAR STRUCTURE

ABSTRACT OF THE DISCLOSURE

A method, system, and computer program product are provided to develop a residue fingerprint for a molecular structure (such as a ligand). Based on the residues of a reference structure (such as a protein), a residue fingerprint defines a set of residues that interacts with the molecular structure. Residue fingerprints can be used to compare different poses of a molecular structure with a reference pose of the same molecular structure, poses of different molecular structures, and/or a different reference three-dimensional structure. Fingerprints are used to define the similarity of structures in terms of binding mode, identify molecules with similar binding modes, or select a subset of molecules that represent the full diversity of binding modes in a larger set. Fingerprints are computed by a van der Waals-based process, and expressed as a list of interacting residues or a binary string representation.